QM/MM Modeling of Catalytic Reactions: Developments and Applications

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In the first part of my talk, I will discuss the development of GULP-CPMD interface program for carrying out hybrid quantum mechanical/polarized-molecular mechanical molecular dynamics (MD) simulations of periodic systems. I will demonstrate that this program is efficient in simulating chemical reactions in zeolites. The second part of my talk will be on the application of QM/MM-MD techniques in predicting the mechanism of antibiotic resistance by class C betalacatamse. This work sheds light on the molecular details of the reaction mechanism, especially the role of various amino acids and drug-protein interaction. My talk will emphasize on the importance of combining rare-event sampling algorithms with QM/MM-MD approaches and high-performance computing in addressing grand challenging problems in chemistry and biology.